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Identification of selective lead compounds for cancer therapy

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Breast cancer is the second most common type of cancer in the World; therefore development of drugs against is of great importance. Although BRCA1 and BRCA2 are the major genes which are responsible for hereditary breast cancer but still there are other genes whose up-regulation can uplift the chances of breast cancer, Homeobox B9 (HOXB9) is a gene, known as persuading agent of lung metastasis, tumor angiogenesis and invasion in breast cancer. 3D structure of HOXB9 wasn't available in Protein Data Bank, hence it was predicted using all three approaches of 3D modeling; Homology modeling, Threading and ab-initio modeling whilst the best compound was chosen by using SAVES server. The best model was then used for docking analysis for which 1000 phytochemicals were docked. Top ten compounds were selected on the basis of lower binding energies and more interacting residues involved. Lys 187, Tyr 192 and Gln 228 were found to be the most active residues in the HOXB9. These top ten compounds were then subjected to drug likeness followed by ADMET analysis via SwissADME software. SwissADME results showed that out of ten compounds only four (PubChem id: 5481218, 42608061, 46880203 and 471695) followed Lipinski rule of five. Thus these compounds could be used as a potential inhibitors of HOXB9, hence suppressing its production in the body. Further in vitro and in vivo studies are required to validate the efficacy of these compounds against HOXB9.